Figure S-5. Large spatial analyses of OKA-III using the SEM and ims 7F-GEO from analytical session 4.6. Symbols are similar to those described on Figure 5.

Figure S-6. Dimer Formation as a Function of Energy Filtering Using the NanoSIMS-50L.

Table S-1. ims 7F-GEO spatial analyses data on OKA-II and III (see Figures 6, S-1, S-4, and S-5).

spot no.	SEM BE intensity	$^{88}Sr/^{42}Ca$	*2σ*	$^{24}Mg/^{42}Ca$	*2σ*	$^{138}Ba/^{42}Ca$	*2σ*
			Holder-II, session-3.8				
1	med	2.3897	0.0162	0.2022	0.0026	0.1502	0.0014
2	d-s	2.0680	0.0846	0.1892	0.0033	0.0371	0.0013
3	med	2.1013	0.0181	0.2126	0.0021	0.1029	0.0011
4	med	2.2125	0.0210	0.2085	0.0025	0.1099	0.0012
5	mtrx	2.3807	0.0155	0.1971	0.0027	0.1483	0.0012
6	mtrx	2.3883	0.0160	0.1970	0.0027	0.1466	0.0012
7	mtrx	2.3859	0.0256	0.1989	0.0028	0.1461	0.0017
8	mtrx	2.3983	0.0236	0.1977	0.0142	0.1448	0.0016
9	mtrx	2.3879	0.0220	0.2012	0.0039	0.1490	0.0027
10	mtrx	2.3777	0.0168	0.1979	0.0030	0.1480	0.0015
11	mtrx	2.4021	0.0208	0.1991	0.0027	0.1474	0.0015
12	med	2.1328	0.0148	0.2092	0.0031	0.1124	0.0014
13	med	2.0663	0.0222	0.2236	0.0027	0.1059	0.0013
14	med	1.8976	0.0172	0.2256	0.0028	0.0899	0.0007
15	med	2.3140	0.0212	0.2169	0.0039	0.1430	0.0016
16	d-s	1.3944	0.0200	0.2186	0.0023	0.0474	0.0006
17	med	2.0212	0.0146	0.2207	0.0029	0.0966	0.0005
18	med	2.2105	0.0189	0.2144	0.0027	0.1168	0.0011
19	mtrx	2.3762	0.0154	0.1963	0.0019	0.1446	0.0008
20	mtrx	2.3844	0.0508	0.1989	0.0063	0.1446	0.0050
mean	*in mtrx*	*2.3868*		*0.1982*		*0.1466*	
stdev %	*in mtrx*	*0.37*		*0.74*		*1.15*	
$2\sigma^{external}$ *%*	*in mtrx*	*0.24*		*0.49*		*0.77*	
			Holder-II, session-4.4				
1	mtrx	2.3068	0.0279	0.2129	0.0027	0.1360	0.0017
2	d-s, incl., hole	1.4937	0.0159	0.2146	0.0030	0.0422	0.0006
3	mtrx	2.2940	0.0215	0.2135	0.0026	0.1341	0.0016
4	barite inclusion	2.0456	0.0185	0.2144	0.0023	0.4391	0.0086
5	d-s, hole	2.1696	0.0168	0.2122	0.0037	0.1240	0.0013
6	med	2.1507	0.0184	0.2156	0.0035	0.1019	0.0011
7	mtrx	2.1370	0.0155	0.2557	0.0030	0.1327	0.0011
8	incl.	2.1836	0.0210	0.2321	0.0037	0.1199	0.0017
9	d-s, crack	1.0879	0.0092	0.2062	0.0032	0.0201	0.0002
10	med	2.0196	0.0203	0.2200	0.0033	0.0817	0.0013
			Holder-II, session-4.5				
1	mtrx	2.3834	0.0166	0.2020	0.0024	0.1434	0.0012
2	mtrx	2.3665	0.0215	0.2024	0.0025	0.1420	0.0011
3	mtrx	2.3659	0.0201	0.2041	0.0024	0.1428	0.0012
4	mtrx	2.3630	0.0191	0.2047	0.0023	0.1422	0.0016
5	med	2.2182	0.0196	0.2180	0.0021	0.1180	0.0012
6	mtrx	2.3895	0.0110	0.2006	0.0022	0.1467	0.0010

7	mtrx	2.3605	0.0238	0.2034	0.0023	0.1404	0.0015
8	mtrx	2.3582	0.0277	0.2022	0.0033	0.1417	0.0014
9	d-l	2.3273	0.0222	0.2058	0.0026	0.1407	0.0017
10	med	2.1613	0.0230	0.2547	0.0035	0.1330	0.0017
11	d-l, bright	2.2311	0.0212	0.2580	0.0046	0.1416	0.0016
12	bright	2.2429	0.0216	0.2287	0.0029	0.1452	0.0016
13	mtrx	2.3522	0.0169	0.2046	0.0036	0.1396	0.0013
14	mtrx	2.3447	0.0265	0.2049	0.0026	0.1425	0.0018
15	d-s	2.2459	0.0208	0.2206	0.0024	0.1315	0.0016
16	med	1.9510	0.0168	0.2129	0.0035	0.0826	0.0009
17	med	1.8827	0.0134	0.2415	0.0037	0.0616	0.0007
18	d-s	2.3551	0.0239	0.2065	0.0033	0.1407	0.0018
19	d-s, incl.	2.2800	0.0266	0.2179	0.0036	0.1521	0.0029
20	mtrx	2.3474	0.0196	0.2056	0.0041	0.1389	0.0015
21	d-s, incl.	1.9111	0.0151	0.2024	0.0029	0.0625	0.0007
22	mtrx	2.3140	0.0198	0.2059	0.0031	0.1391	0.0015
23	d-s, incl.	2.1851	0.0174	0.2050	0.0035	0.1458	0.0089
mean	*in matrix*	*2.3587*		*0.2037*		*0.1417*	
stdev %	*in matrix*	*0.85*		*0.83*		*1.59*	
$2\sigma^{external}$ %	*in matrix*	*0.26*		*0.25*		*0.48*	
			Holder-III, session-4.6				
1	mtrx	2.2858	0.0213	0.2173	0.0038	0.1346	0.0015
2	mtrx	2.2827	0.0163	0.2139	0.0029	0.1348	0.0013
3	mtrx	2.2927	0.0174	0.2151	0.0025	0.1350	0.0011
4	med	2.2822	0.0172	0.2168	0.0026	0.1341	0.0015
5	dark	1.6465	0.0157	0.2494	0.0042	0.1882	0.0097
6	dark	1.8208	0.0218	0.2172	0.0030	0.0559	0.0004
7	dark	1.4084	0.0133	0.2292	0.0033	0.0214	0.0003
8	dark	1.8352	0.0175	0.2267	0.0032	0.0795	0.0012
9	d-s	1.6736	0.0158	0.2302	0.0040	0.0347	0.0005
10	med	2.3079	0.0230	0.2244	0.0035	0.1198	0.0015
mean	*in matrix*	2.287067		0.215433		0.1348	
stdev %	*in matrix*	0.22		0.80		0.15	
$2\sigma^{external}$ %	*in matrix*	0.26		0.92		0.17	

$2\sigma_{88/42}$, $2\sigma_{24/42}$, and $2\sigma_{138/42}$ are the doubled internal standard errors between 151 and 200 cycles of particular spot;
mtrx – homogeneous calcite matrix; med – calcite with medium BE intensity; d-s and d-l – dark spots and lines; bright – brightest calce area; incl. – Sr-Ba sulfate or Sr-Ca carbonate inclusions. The standard deviation and external 2σ calculated in data sets with significant number of the SIMS spots collected in the matrix.

Table S-2. ims 7F-GEO spatial analyses data on BlueCC, NBS-19, and 135CC (holder-II, session 3.8, see Figure 8)

Spot #	*$^{88}Sr/^{42}Ca$*	*2σ*	*$^{24}Mg/^{42}Ca$*	*2σ*	*$^{138}Ba/^{42}Ca$*	*2σ*
			BlueCC-II			
1	0.0764	0.0020	0.1486	0.0026	5.88E-04	6.06E-05
2	0.0759	0.0012	0.1431	0.0027	5.42E-04	5.92E-05
3	0.0754	0.0021	0.1454	0.0021	5.67E-04	4.88E-05
4	0.0741	0.0020	0.1459	0.0029	5.34E-04	4.94E-05
5	0.0760	0.0013	0.1431	0.0017	5.58E-04	5.42E-05
6	0.0711	0.0018	0.1449	0.0021	5.12E-04	5.63E-05
7	0.0765	0.0019	0.1466	0.0029	5.95E-04	7.99E-05
8	0.0758	0.0011	0.1496	0.0025	5.58E-04	1.65E-05
mean	*0.0751*		*0.1459*		*5.57E-04*	
stdev %	*2.39*		*1.60*		*4.93*	
$2\sigma^{external}$ %	*1.69*		*1.13*		*3.49*	
			NBS-19			
1	0.0244	0.0012	0.7399	0.007	9.51E-05	1.96E-05
2	0.0258	0.0012	0.741	0.0054	1.29E-04	2.52E-05
3	0.0236	0.0009	0.7607	0.0095	1.01E-04	1.49E-05
4	0.0256	0.0010	0.7425	0.0104	1.18E-04	2.31E-05
5	0.0254	0.0014	0.6702	0.0041	9.55E-05	2.09E-05
6	0.0259	0.0008	0.768	0.0061	1.45E-04	2.29E-05
7	0.0243	0.0009	0.7672	0.0054	1.13E-04	2.68E-05
mean	*0.0250*		*0.741357*		*1.14E-04*	
stdev %	*3.57*		*4.55*		*16.33*	
$2\sigma^{external}$ %	*2.70*		*3.44*		*12.34*	
			135CC			
1	0.0298	0.0016	6.09E-03	4.59E-04	3.26E-05	1.26E-05
2	0.0251	0.0013	4.40E-03	3.27E-04	3.08E-05	7.48E-06
3	0.0073	0.0006	4.94E-03	2.50E-04	2.90E-05	1.16E-05
4	0.0135	0.0009	4.06E-03	3.67E-04	1.71E-05	1.16E-05
5	0.0223	0.0012	4.17E-03	2.76E-04	4.31E-05	1.38E-05
6	0.0257	0.0012	3.68E-03	3.48E-04	1.52E-05	8.25E-06
7	0.0203	0.0012	3.87E-03	3.35E-04	2.84E-05	1.61E-05
8	0.0262	0.0012	5.37E-03	4.54E-04	3.23E-05	9.82E-06
mean	*0.0213*		*4.57E-03*		*2.86E-05*	
stdev %	*34.99*		*18.14*		*31.22*	
$2\sigma^{external}$ %	*24.74*		*12.83*		*22.08*	

$2\sigma_{88/42}$, $2\sigma_{24/42}$, and $2\sigma_{138/42}$ are the doubled internal standard errors between 151 and 200 cycles of particular spot

Table S-3. Averaged ims 7F-GEO data of the single crystal of BlueCC-III. The data collected at different sessions and normalized to OKA-III (see Figure 10).

session	*n*	Sr/Ca	*2σ*	Mg/Ca	*2σ*	Ba/Ca	*2σ*
1	5	0.5787	0.0041	8.1574	0.0361	9.13E-03	1.59E-04
2	6	0.5762	0.0021	8.4245	0.0488	9.20E-03	0.99E-04
3.1	6	0.5756	0.0074	8.2999	0.0597	9.30E-03	2.82E-04
3.2	4	0.5702	0.0041	8.1261	0.0532	9.08E-03	0.89E-04
3.3	3	0.5676	0.0057	8.2331	0.0873	8.89E-03	5.17E-04
3.4	4	0.5674	0.0063	8.3286	0.2883	9.47E-03	3.02E-04
3.5	5	0.5699	0.0048	8.2449	0.2247	9.11E-03	3.25E-04
3.6	2	0.5752	0.0198*	8.1791	0.1208*	8.76E-03	1.73E-04
3.7	2	0.5766	0.0088*	8.1247	0.1548*	9.21E-03	1.90E-04
3.8	2	0.5791	0.0024*	8.1167	0.0593*	8.85E-03	0.43E-04
4.1	2	0.5725	0.0136*	8.2019	0.0647*	9.17E-03	0.39E-04
4.2	1	0.5756	0.0010[#]	8.2099	0.0209[#]	9.01E-03	3.19E-04

n is the number of analyzed spots in the particular sub-session;
$2\sigma_{88/42}$, $2\sigma_{24/42}$, and $2\sigma_{138/42}$ are the doubled external standard errors between *n* spots;
* - the errors are expressed as the difference between two ratio values;
[#] - the error is an internal 2σ from a cycles of a single spot;
BlueCC-III: Sr/Ca=0.578 and Mg/Ca=8.047 mmol/mol; values are from ICP-MS data of BlueCC-I;
OKA-III: Sr/Ca=18.816 and Mg/Ca=4.885 mmol/mol; values are from ICP-MS data of OKA-I;
For OKA's Ba/Ca the literature value of 1.61 mmol/mol was assumed (see Gaetani and Cohen 2006).
For description of the calculations please see Appendix 4, equation 4.1.

Table S-4. Calibration of ims 7F-GEO versus ICP-MS data (see Figure 12).

name	*n*	*Sr/Ca ICP-MS*	*$^{88}Sr/^{42}Ca$ 7F-GEO*	*2σ*	*Mg/Ca ICP-MS*	*$^{24}Mg/^{42}Ca$ 7F-GEO*	*2σ*
			Holder-II, session 3.8,				
BlueCC	8	0.6086(5)	0.0752	0.0013	3.5551(1540)	0.1459	0.0017
OKA(mtrx)	11	18.9603(7476)	2.4086	0.0073	4.7785(1654)	0.1960	0.0010
NBS-19	7	0.1912*	0.0250	0.0007	17.7175*	0.7419	0.0255
			Holder-I, session 4.2,				
BlueCC	2	0.6057(5)	0.0731	0.0011	3.7455(1540)	0.1626	0.0003
OKA(mtrx)	1	19.0010(7476)	2.3597	0.0195	4.8607(1654)	0.2084	0.0021
UCI	1	0.2043(4)	0.0253	0.0004	3.4461(166)	0.1514	0.0014
RPI	1	0.0330(4)	0.0045	0.0004	0.3960(103)	0.0197	0.0006
Las-20	2	0.5148(163)	0.0580	0.0001	46.3109(1.7408)	2.1766	0.0344
135CC	2	0.2363(48)	0.0287	0.0005	0.0732(16)	0.0056	0.0005
HUJ	2	8.2635(89)	0.9449	0.0209	0.0214(109)	0.0068	0.0044
			Holder-I, session 4.3				
BlueCC	3	0.6057(5)	0.0691	0.0022	3.7455(1540)	0.1673	0.0031
OKA(mtrx)	2	19.0010(7476)	2.2874	0.0044	4.8607(1654)	0.2135	0.0002
HUJ	2	8.2096(854)	0.9275	0.0079	0.0214(109)	0.0045	0.0011

The elemental ratios in holder-I (mmol/mol) were determined by ID-ICP-MS. Units in parentheses represent the error in terms of least units cited. Therefore, 0.6083(4) should be read as 0.6083±0.0004. This error is the half of the difference between highest and lowest values measured in different crystals of the single cleavage fragment. The elemental ratios of the standards from holder-II were calculated by comparison with those from holder-I using IMS-7, for example see Appendix 4 (equation 4.1). The errors related to ICP-MS analysis of OKA and BlueCC from holder-II exceed those from SIMS measurements. Therefore, errors remained unchanged from those evaluated by ICP-MS analysis.

The isotopic ratios (cps/cps) were determined by ims 7F-GEO. Each standard was analyzed with number of *n* spots.

2σ is the doubled external standard error between multiple analyses of particular standard during session 3.8; it is doubled internal standard error when n=1 in the session 4.2; it is also the half of the data range when n=2 or 3 in the sessions 4.2 and 4.3.

Ratios and errors for OKA were calculated from the data collected on matrix area only. Some data points were excluded from the Table, because termination of Duoplasmatron.

(*) – only single ICP-MS measurement was performed on NBS-19, therefore no errors are presented for Sr/Ca and Mg/Ca

Table S-5. NanoSIMS-50L spatial analyses data on OKA-II and BlueCC-II, session 2.1 (Figures 7 and 9).

spot no.	$^{88}Sr/^{42}Ca$	2σ	$^{24}Mg/^{42}Ca$	2σ	$^{138}Ba/^{42}Ca$	2σ
			OKA-II			
1	1.9213	0.0132	0.1829	0.0026	0.1246	0.0023
2	1.7222	0.0122	0.1869	0.0021	0.0857	0.0015
3	1.4710	0.0113	0.2050	0.0029	0.0691	0.0014
4	1.8122	0.0119	0.1863	0.0023	0.0950	0.0017
5	1.9294	0.0103	0.1863	0.0023	0.1263	0.0020
6	1.9172	0.0098	0.1874	0.0021	0.1241	0.0020
7	1.9019	0.0113	0.1869	0.0026	0.1238	0.0021
8	1.9269	0.0096	0.1834	0.0024	0.1240	0.0019
9	1.9139	0.0115	0.1868	0.0021	0.1227	0.0021
10	1.9302	0.0127	0.1886	0.0028	0.1252	0.0018
mean mtrx	*1.9201*		*0.1860*		*0.1244*	
stdev %	*0.53*		*1.13*		*0.91*	
$2\sigma^{external}$ *%*	*0.20*		*0.43*		*0.35*	
			BuleCC-II			
1	6.76E-02	1.58E-03	0.1483	0.0011	1.71E-03	2.65E-04
2	6.68E-02	1.55E-03	0.1551	0.0014	1.91E-03	2.39E-04
3	6.59E-02	1.64E-03	0.1543	0.0013	1.62E-03	2.34E-04
4	6.85E-02	1.36E-03	0.1514	0.0014	1.59E-03	2.28E-04
5	6.81E-02	1.66E-03	0.1514	0.0013	1.66E-03	2.18E-04
6	7.05E-02	1.26E-03	0.1546	0.0026	1.93E-03	2.35E-04
7	6.66E-02	1.47E-03	0.1548	0.0026	1.82E-03	2.37E-04
8	6.73E-02	1.38E-03	0.1543	0.0025	1.76E-03	2.09E-04
9	6.64E-02	1.75E-03	0.1552	0.0025	1.75E-03	2.40E-04
10	6.71E-02	1.66E-03	0.1497	0.0026	1.75E-03	2.48E-04
mean	*0.0675*		*0.1529*		*1.75E-03*	
stdev %	*1.95*		*1.64*		*6.47*	
$2\sigma^{external}$ *%*	*0.62*		*0.52*		*2.04*	

$2\sigma_{88/42}$, $2\sigma_{24/42}$, and $2\sigma_{138/42}$ are the doubled internal standard errors between 151 and 200 cycles of particular spot

Table S-6. Averages of the BlueCC NanoSIMS-50L data collected at different sessions and normalized to OKA or NBS-19, or both (see Figure 11).

session	n	Sr/Ca	$2\sigma_{Sr/Ca}$	Mg/Ca	$2\sigma_{Mg/Ca}$	Ba/Ca	$2\sigma_{Ba/Ca}$
1.1	4	0.5842	0.0026	8.5346	0.1511	4.70E-03	1.41E-04
1.2	6	0.5414	0.0034	8.5851	0.0180	4.42E-03	2.22E-04
2.1	10	0.6814	0.0085	3.7717	0.0389	2.27E-02	9.33E-04
2.2	3	0.6542	0.0477	3.4964	0.1644	8.67E-03	5.34E-03
2.3	3	0.6725	0.0381	3.4002	0.4986	8.67E-03	8.19E-04
2.4	6	0.5908	0.0061	7.8784	0.1195	1.18E-02	8.97E-04
3.1	10	0.5711	0.0072	8.6376	0.0444	3.42E-02	3.16E-03
4.1[#]	1	0.5878	0.0006	3.8521	0.0145	n/a	n/a
4.2	3	0.6032	0.0083	3.4538	0.0025	n/a	n/a

n is the number of analyzed spots in the particular sub-session;
2σ is the doubled external standard error between analyses performed at particular date.
[#] - the error is an internal 2σ from a cycles of a single spot.
Sessions 1.1 and 1.2: BlueCC-IV normalized to NBS-19;
Sessions 2.3, and 2.4: BlueCC-IV normalized to OKA-IV;
Sessions 2.1-2.3: BlueCC-II normalized to OKA-II;
Sessions 4.1 and 4.2: BlueCC-I normalized to OKA-I.
BlueCC-I (directly measured with ICP-MS): Sr/Ca=0.6057 and Mg/Ca=3.7455 mmol/mol;
BlueCC-II (based on BlueCC-I by ims 7F-GEO): Sr/Ca=0.6086 and Mg/Ca=3.5551 mmol/mol;
BlueCC-IV (based on BlueCC-I by ims 7F-GEO): Sr/Ca=0.5967 and Mg/Ca=8.5991 mmol/mol;
OKA-I (directly measured with ICP-MS): Sr/Ca=19.0010 and Mg/Ca=4.8607 mmol/mol;
OKA-II (based on OKA-I by ims 7F-GEO): Sr/Ca=19.3901 and Mg/Ca=4.5890 mmol/mol;
OKA-IV (based on OKA-I by ims 7F-GEO): Sr/Ca=18.9887 and Mg/Ca=4.6950 mmol/mol.
For OKA's Ba/Ca the literature value of 1.61 mmol/mol was assumed (see Gaetani and Cohen 2006).
For description of the calculations please see Appendix 4, equation 4.1.

Table S-7. Calibration of NanoSIMS-50L versus ICP-MS data (also see Figure 12). The used cycles are 151-200, except session 4.2 (41-120 cycles) (see Figure 13).

name	*n*	*Sr/Ca*	*$^{88}Sr/^{42}Ca$*	*2σ*	*Mg/Ca*	*$^{24}Mg/^{42}Ca$*	*2σ*
		ICP-MS	*NanoSIMS*		*ICP-MS*	*NanoSIMS*	
			Holder IV, session 1.1				
BlueCC	4	0.5967(41)	0.0723	0.0003	8.5991(1540)	0.2225	0.0039
AG-1	2	9.6(4)	1.1052	0.0297	0.27(11)	0.0065	0.0017
NBS-19	4	0.1912*	0.0237	0.0009	17.7175*	0.4619	0.0074
			Holder II, session 2.2				
BlueCC	3	0.6086(5)	0.0784	0.0007	3.5551(1540)	0.1040	0.0041
NBS-19	3	0.1912*	0.0258	0.0021	17.7175*	0.4975	0.0238
OKA-II	3	18.9603(5)	2.3687	0.0435	4.7785 (1654)	0.1460	0.0170
			Holder IV, session 2.4				
BlueCC	6	0.5967(41)	0.0795	0.0008	8.5991 (1540)	0.2030	0.0031
AG-1	6	9.6(4)	1.2266	0.0018	0.27(11)	0.0022	0.0011
OKA	6	18.5677(7476)	2.5243	0.0149	4.8888(1654)	0.1238	0.0029
			Holder IV, session 3.1				
BlueCC	10	0.5967(41)	0.0632	0.0008	8.5991(1540)	0.278	0.0014
AG-1	5	9.6(4)	0.9680	0.0139	0.27(11)	0.0017	0.0003
NBS	6	0.1912*	0.0206	0.0009	17.7175*	0.5875	0.0186
OKA	6	18.5677(7476)	2.0401	0.0368	4.8888(1654)	0.1510	0.0080
			Holder I, session 4.1 #				
BlueCC	1	0.6057(5)	0.0646	0.0012	3.7455(1540)	0.1333	0.0017
OKA	1	19.0010(7476)	2.0883	0.0127	4.8607(1654)	0.1682	0.0022
UCI	1	0.2043(4)	0.0220	0.0007	3.4461(166)	0.1267	0.0018
RPI	1	0.0330(4)	0.0045	0.0003	0.3960(103)	0.0155	0.0005
LAS-20	1	0.5148(163)	0.0469	0.0010	45.3109(1.7408)	1.7518	0.0114
HUJ	1	8.2635(89)	0.8588	0.0058	0.0214(109)	0.0012	0.0002
HUJ	1	8.2635(89)	0.8196	0.0050	0.0214(109)	0.0032	0.0003
1355CC	1	0.2363(48)	0.0262	0.0008	0.0732(16)	0.0072	0.0004
1355CC	1	0.2363(48)	0.0222	0.0007	0.0732(16)	0.1288	0.0017
			Holder I, session 4.2, cycles 41-120				
BlueCC	3	0.6057(5)	0.0422	0.0006	3.7455(1540)	0.1867	0.0001
OKA	4	19.001(7476)	1.3293	0.0470	4.8607(1654)	0.2628	0.0103
UCI	4	0.2043(4)	0.0149	0.0005	3.4461(166)	0.1887	0.0080
RPI	4	0.0330(4)	0.0030	0.0001	0.3960(103)	0.0209	0.0012
LAS-20	4	0.5148(163)	0.0342	0.0006	45.3109(1.7408)	2.5896	0.0380
HUJ-I	3	8.2635(89)	0.5392	0.0259	0.0214(109)	0.0048	0.0029
135CC-I	3	0.2363(48)	0.0170	0.0006	0.0732(16)	0.0125	0.0018

The elemental ratios in holder-I (mmol/mol) were determined by ID-ICP-MS. Units in parentheses represent the half of the difference between highest and lowest measured values. Sr/Ca and Mg/Ca ratios and errors in OKA and BlueCC from other holders were calculated similarly as in Table 6 (also see Appendix 3, equation 3.1). The errors related to ICP-MS analysis of OKA and BlueCC from other holder exceed those came from SIMS measurements in most cases. The only exceptions are Sr/Ca in BlueCC-III and IV, where presented errors are related to SIMS measurements; all other elemental errors are related were evaluated from ICP-MS analyses of standards from holder-I. The ICP-MS analyses of AG-1 were performed by Glenn Gaetani at WHOI, the units in parentheses represent the standard deviations of total nine measurements in three crystals (3 data per each crystal).

Isotopic ratios (cps/cps) were determined by NanoSIMS-50L. Each standard was analyzed with number of *n* spots.

2σ is the doubled external standard error between multiple analyses of particular standard during single sub-session; it is doubled internal standard error when n=1 in the session 4.1; it is also the half of the data range when n=2 in the sessions 1.1

and 2.2. Ratios and errors for OKA were calculated from the data collected on matrix area only. HUJ and 135CC are heterogeneous in $^{24}Mg/^{42}Ca$ (see session 4.1), therefore two single data points of each standard are presented instead of its mean values. Some data points were excluded from the Table, because termination of Duoplasmatron.
(*) – only single ICP-MS measurement was performed on NBS-19, therefore no errors are presented for Sr/Ca and Mg/Ca;
(#) – here 2σ of NanoSIMS-50L intensity ratios correspond to the internal precision, because n=1.

Table S-8. ID-ICP-MS data (see Figure 4)

name	*crystal #*	*Sr/Ca mmol/mol*	*Mg/Ca mmol/mol*
OKA-2*	1	19.4317	4.6684
OKA-3*	1	19.5332	4.9146
OKA-5*	1	18.0380	4.9991
OKA	2	18.9513	4.9711
OKA-1	3	16.8505	5.2955
OKA-1	4	18.7387	4.7035
Int./2 % cr-1		*3.93*	*3.30*
Int./2 % all cr.		*7.21*	*3.01*
Stdev % all cr.		*5.42*	*2.31*
BlueCC -2*	1	0.6055	3.6184
BlueCC -3*	1	0.6053	3.6915
BlueCC -4*	1	0.6062	3.926
BlueCC -6	2	0.6084	3.9850
BlueCC -7	2	0.6086	3.9477
BlueCC	3	0.6031	3.5908
BlueCC	4	0.5456	5.3256
Int./2 % cr-1		*0.07*	*4.11*
Int./2 % cr-2		*0.01*	*0.47*
Int./2 % all cr.		*5.27*	*21.27*
Stdev % all cr.		*3.85*	*15.48*
NBS-19	powder	0.1912	17.717
135CC-2*	1	0.2315	0.0748
135CC-3*	1	0.2410	0.0715
135CC-5	2	0.2128	0.0544
135CC	3	0.1368	0.0838
Int./2 % cr-1		*2.01*	*2.21*
Int./2 % all cr.		*25.35*	*20.60*
Stdev % all cr.		*23.01*	*17.27*
HUJ-1*	1	8.2724	0.0313
HUJ-4*	1	8.2546	0.0095
HUJ-5*	1	8.1016	0.0234
Int./2 % cr-1		*1.04*	*255.82*
LAS20-2*	1	0.5001	47.0329
LAS20-3*	1	0.5115	45.3487
LAS20-5	1	0.5327	43.5512
LAS-20	2	0.4603	44.1062
Int./2 % cr-1		*3.17*	*3.84*

Int./2 % all cr.		*5.11*	*3.25*
Stdev % all cr.		*6.07*	*3.43*
RPI-2*	1	0.0327	0.3893
RPI-3*	1	0.0329	0.4096
RPI-5*	1	0.0334	0.3891
RPI-cal	2	0.0337	0.3845
Int./2 % cr-1		*1.07*	*2.60*
Int./2 % all cr.		*1.54*	*3.20*
Stdev % all cr.		*1.41*	*2.86*
UCI-2*	1	0.2039	3.4616
UCI-4*	1	0.2047	3.4485
UCI-5*	1	0.2042	3.4283
Int./2 % cr-1		*0.20*	*0.48*
AG-1	a few cr.	9.6	0.27
Stdev% all cr.		*4.2*	*40.7*

The same crystal numbers correspond to analyses of broken pieces of the single crystal. Internal errors are less than 1 ‰. The numbers by the standard name are for ICP-MS analyses only and are not used in the manuscript.
Int./2 is the data range divided by two;
(*) – the adjacent piece to those, which was analyzed with ims 7F-GEO and NanoSIMS-50L; if more than one star is presented for the same standard then the average Sr/Ca and Mg/Ca were used.
The following Me/Ca ratios (mmol/mol) were determined with ICP-MS in other SIMS studies:
OKA: Sr/Ca=19.30 and Mg/Ca=4.47 (Gaetani and Cohen, 2006)
BlueCC: Sr/Ca=0.56 (Hart and Cohen, 1996; Heikoop et al., 2002)
NBS-19: Sr/Ca=0.199 and Mg/Ca=13.04 (Sano et al., 2005)
LAS-20: Sr/Ca=0.595 and Mg/Ca=31.1 (Sano et al., 2005)

Table S-9. EMP data of inclusions in OKA in wt%.

Spot#	structure	CaO	SrO	BaO	SO_3	Na_2O	La_2O	Ce_2O	Total
				Holder-II					
35	barite	0.89	43.71	13.02	39.81	n/d	n/d	2.55	100%
36	aragonite	13.01	42.67	1.56	n/d	3.76	3.73	4.88	99.74
				Holder-III					
37	barite	1.46	0.12	57.00	29.95	0.10	n/d	11.37	100%
38	aragonite	19.21	35.54	2.12	n/d	4.00	3.29	4.99	99.21
39	aragonite	13.89	40.22	1.03	n/d	4.60	2.85	3.56	96.22
40	aragonite	15.21	36.01	7.81	0.12	3.98	2.23	3.71	99.29
				Holder-V					
41	aragonite	15.40	41.41	3.64	n/d	2.93	3.14	4.41	101.04
42	aragonite	13.57	32.79	12.00	n/d	3.69	3.24	5.61	100.93

Structure was determined by EBSD and confirmed with micro-Raman for barite.
No Mg, Si, K, Al, or Yb were detected.
Totals for carbonate inclusions were calculated assuming $30CO_2$.
Oxides concentrations in the sulfate inclusions were normalized to 100%.